Frank NoÃ©

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9177783/publications.pdf

Version: 2024-02-01

149 papers	15,875 citations	23565 58 h-index	19188 118 g-index
170 all docs	170 docs citations	170 times ranked	10066 citing authors

#	Article	IF	Citations
1	Generating stable molecules using imitation and reinforcement learning. Machine Learning: Science and Technology, 2022, 3, 015008.	5.0	4
2	Deeptime: a Python library for machine learning dynamical models from time series data. Machine Learning: Science and Technology, 2022, 3, 015009.	5.0	37
3	Identifying optimal cycles in quantum thermal machines with reinforcement-learning. Npj Quantum Information, 2022, 8, .	6.7	57
4	Roadmap on Machine learning in electronic structure. Electronic Structure, 2022, 4, 023004.	2.8	69
5	A litmus test for classifying recognition mechanisms of transiently binding proteins. Nature Communications, 2022, 13, .	12.8	13
6	Molecular mechanism of inhibiting the SARS-CoV-2 cell entry facilitator TMPRSS2 with camostat and nafamostat. Chemical Science, 2021, 12, 983-992.	7.4	66
7	Discovery of a hidden transient state in all bromodomain families. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	24
8	Synergistic inhibition of SARS-CoV-2 cell entry by otamixaban and covalent protease inhibitors: pre-clinical assessment of pharmacological and molecular properties. Chemical Science, 2021, 12, 12600-12609.	7.4	11
9	Neural mode jump Monte Carlo. Journal of Chemical Physics, 2021, 154, 074101.	3.0	4
10	Camostat mesylate inhibits SARS-CoV-2 activation by TMPRSS2-related proteases and its metabolite GBPA exerts antiviral activity. EBioMedicine, 2021, 65, 103255.	6.1	256
11	Convergence to the fixed-node limit in deep variational Monte Carlo. Journal of Chemical Physics, 2021, 154, 124108.	3.0	13
12	TorchMD: A Deep Learning Framework for Molecular Simulations. Journal of Chemical Theory and Computation, 2021, 17, 2355-2363.	5.3	101
13	What Markov State Models Can and Cannot Do: Correlation versus Path-Based Observables in Protein-Folding Models. Journal of Chemical Theory and Computation, 2021, 17, 3119-3133.	5.3	32
14	Multi-body effects in a coarse-grained protein force field. Journal of Chemical Physics, 2021, 154, 164113.	3.0	28
15	Unsupervised Learning Methods for Molecular Simulation Data. Chemical Reviews, 2021, 121, 9722-9758.	47.7	182
16	Independent Markov decomposition: Toward modeling kinetics of biomolecular complexes. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	11
17	Symmetric and antisymmetric kernels for machine learning problems in quantum physics and chemistry. Machine Learning: Science and Technology, 2021, 2, 045016.	5.0	9
18	Machine learning implicit solvation for molecular dynamics. Journal of Chemical Physics, 2021, 155, 084101.	3.0	35

#	Article	IF	Citations
19	Multiscale molecular kinetics by coupling Markov state models and reaction-diffusion dynamics. Journal of Chemical Physics, 2021, 155, 124109.	3.0	13
20	Hydrodynamic coupling for particle-based solvent-free membrane models. Journal of Chemical Physics, 2021, 155, 114108.	3.0	5
21	Parameterized Hypercomplex Graph Neural Networks for Graph Classification. Lecture Notes in Computer Science, 2021, , 204-216.	1.3	9
22	Alpha 1 Antitrypsin is an Inhibitor of the SARS-CoV-2â€“Priming Protease TMPRSS2. Pathogens and Immunity, 2021, 6, 55-74.	3.1	73
23	Thermodynamics and Kinetics of Aggregation of Flexible Peripheral Membrane Proteins. Journal of Physical Chemistry Letters, 2021, 12, 10497-10504.	4.6	12
24	Progress in deep Markov state modeling: Coarse graining and experimental data restraints. Journal of Chemical Physics, 2021, 155, 214106.	3.0	10
25	Coupling Particle-Based Reaction-Diffusion Simulations with Reservoirs Mediated by Reaction-Diffusion PDEs. Multiscale Modeling and Simulation, 2021, 19, 1659-1683.	1.6	7
26	Geometrical characterization of T cell receptor binding modes reveals classâ€specific binding to maximize access to antigen. Proteins: Structure, Function and Bioinformatics, 2020, 88, 503-513.	2.6	15
27	Variational Approach for Learning Markov Processes from Time Series Data. Journal of Nonlinear Science, 2020, 30, 23-66.	2.1	156
28	Machine learning for protein folding and dynamics. Current Opinion in Structural Biology, 2020, 60, 77-84.	5.7	116
29	Coarse graining molecular dynamics with graph neural networks. Journal of Chemical Physics, 2020, 153, 194101.	3.0	103
30	Deep-neural-network solution of the electronic SchrÃ¶dinger equation. Nature Chemistry, 2020, 12, 891-897.	13.6	272
31	Neuraldecipher â€“ reverse-engineering extended-connectivity fingerprints (ECFPs) to their molecular structures. Chemical Science, 2020, 11, 10378-10389.	7.4	28
32	grÃ¼nifai: interactive multiparameter optimization of molecules in a continuous vector space. Bioinformatics, 2020, 36, 4093-4094.	4.1	7
33	Ensemble learning of coarse-grained molecular dynamics force fields with a kernel approach. Journal of Chemical Physics, 2020, 152, 194106.	3.0	38
34	Large-scale simulation of biomembranes incorporating realistic kinetics into coarse-grained models. Nature Communications, 2020, 11, 2951.	12.8	31
35	Coupling of Conformational Switches in Calcium Sensor Unraveled with Local Markov Models and Transfer Entropy. Journal of Chemical Theory and Computation, 2020, 16, 2584-2593.	5.3	12
36	Machine Learning for Molecular Simulation. Annual Review of Physical Chemistry, 2020, 71, 361-390.	10.8	456

#	Article	IF	Citations
37	Machine Learning for Molecular Dynamics on Long Timescales. Lecture Notes in Physics, 2020, , 331-372.	0.7	22
38	Deflation reveals dynamical structure in nondominant reaction coordinates. Journal of Chemical Physics, 2019, 151, .	3.0	12
39	Efficient multi-objective molecular optimization in a continuous latent space. Chemical Science, 2019, 10, 8016-8024.	7.4	143
40	Dynamic graphical models of molecular kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 15001-15006.	7.1	33
41	Structure and assembly of the mitochondrial membrane remodelling GTPase Mgm1. Nature, 2019, 571, 429-433.	27.8	86
42	Polymer-like Model to Study the Dynamics of Dynamin Filaments on Deformable Membrane Tubes. Biophysical Journal, 2019, 117, 1870-1891.	0.5	13
43	Diffusion-influenced reaction rates in the presence of pair interactions. Journal of Chemical Physics, 2019, 151, 164105.	3.0	14
44	Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning. Science, 2019, 365, .	12.6	332
45	Targeted Adversarial Learning Optimized Sampling. Journal of Physical Chemistry Letters, 2019, 10, 5791-5797.	4.6	41
46	Learning continuous and data-driven molecular descriptors by translating equivalent chemical representations. Chemical Science, 2019, 10, 1692-1701.	7.4	293
47	Dynamically Driven Allostery in MHC Proteins: Peptide-Dependent Tuning of Class I MHC Global Flexibility. Frontiers in Immunology, 2019, 10, 966.	4.8	41
48	Variational selection of features for molecular kinetics. Journal of Chemical Physics, 2019, 150, 194108.	3.0	46
49	Identification of kinetic order parameters for non-equilibrium dynamics. Journal of Chemical Physics, 2019, 150, 164120.	3.0	31
50	Machine Learning of Coarse-Grained Molecular Dynamics Force Fields. ACS Central Science, 2019, 5, 755-767.	11.3	306
51	The mechanism of RNA base fraying: Molecular dynamics simulations analyzed with core-set Markov state models. Journal of Chemical Physics, 2019, 150, 154123.	3.0	24
52	ReaDDy 2: Fast and flexible software framework for interacting-particle reaction dynamics. PLoS Computational Biology, 2019, 15, e1006830.	3.2	59
53	Reactive SINDy: Discovering governing reactions from concentration data. Journal of Chemical Physics, 2019, 150, 025101.	3.0	84
54	Cyclization and Relaxation Dynamics of Finite-Length Collapsed Self-Avoiding Polymers. Physical Review Letters, 2019, 122, 067801.	7.8	12

#	Article	IF	Citations
55	Nanoscale coupling of endocytic pit growth and stability. Science Advances, 2019, 5, eaax5775.	10.3	17
56	Markov Models of Molecular Kinetics. Journal of Chemical Physics, 2019, 151, 190401.	3.0	52
57	Kernel methods for detecting coherent structures in dynamical data. Chaos, 2019, 29, 123112.	2.5	17
58	Single event visualization of unconventional secretion of FGF2. Journal of Cell Biology, 2019, 218, 683-699.	5.2	39
59	OpenPathSampling: A Python Framework for Path Sampling Simulations. 2. Building and Customizing Path Ensembles and Sample Schemes. Journal of Chemical Theory and Computation, 2019, 15, 837-856.	5.3	34
60	OpenPathSampling: A Python Framework for Path Sampling Simulations. 1. Basics. Journal of Chemical Theory and Computation, 2019, 15, 813-836.	5.3	45
61	Porting Adaptive Ensemble Molecular Dynamics Workflows to the Summit Supercomputer. Lecture Notes in Computer Science, 2019, , 397-417.	1.3	5
62	Introduction to Markov state modeling with the PyEMMA software [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	6.4	45
63	Particle-based membrane model for mesoscopic simulation of cellular dynamics. Journal of Chemical Physics, 2018, 148, 044901.	3.0	33
64	Identifying Conformational-Selection and Induced-Fit Aspects in the Binding-Induced Folding of PMI from Markov State Modeling of Atomistic Simulations. Journal of Physical Chemistry B, 2018, 122, 5649-5656.	2.6	24
65	Rapid Calculation of Molecular Kinetics Using Compressed Sensing. Journal of Chemical Theory and Computation, 2018, 14, 2771-2783.	5.3	24
66	A scalable approach to the computation of invariant measures for high-dimensional Markovian systems. Scientific Reports, 2018, 8, 1796.	3.3	6
67	Data-Driven Model Reduction and Transfer Operator Approximation. Journal of Nonlinear Science, 2018, 28, 985-1010.	2.1	192
68	VAMPnets for deep learning of molecular kinetics. Nature Communications, 2018, 9, 5.	12.8	330
69	Time-lagged autoencoders: Deep learning of slow collective variables for molecular kinetics. Journal of Chemical Physics, 2018, 148, 241703.	3.0	283
70	It takes two transducins to activate the cGMP-phosphodiesterase 6 in retinal rods. Open Biology, 2018, 8, .	3.6	34
71	Collective hydrogen-bond rearrangement dynamics in liquid water. Journal of Chemical Physics, 2018, 149, 244504.	3.0	22
72	Reversible Interacting-Particle Reaction Dynamics. Journal of Physical Chemistry B, 2018, 122, 11240-11250.	2.6	27

#	Article	IF	Citations
73	Grand canonical diffusion-influenced reactions: A stochastic theory with applications to multiscale reaction-diffusion simulations. Journal of Chemical Physics, 2018, 149, 044102.	3.0	12
74	Optimal Data-Driven Estimation of Generalized Markov State Models for Non-Equilibrium Dynamics. Computation, 2018, 6, 22.	2.0	20
75	MSM/RD: Coupling Markov state models of molecular kinetics with reaction-diffusion simulations. Journal of Chemical Physics, 2018, 148, 214107.	3.0	25
76	Variational Koopman models: Slow collective variables and molecular kinetics from short off-equilibrium simulations. Journal of Chemical Physics, 2017, 146, 154104.	3.0	100
77	Markov state models from short non-equilibrium simulationsâ€”Analysis and correction of estimation bias. Journal of Chemical Physics, 2017, 146, .	3.0	51
78	The Isomeric Preference of an Atypical Dopamine Transporter Inhibitor Contributes to Its Selection of the Transporter Conformation. ACS Chemical Neuroscience, 2017, 8, 1735-1746.	3.5	31
79	Lipid-mediated PX-BAR domain recruitment couples local membrane constriction to endocytic vesicle fission. Nature Communications, 2017, 8, 15873.	12.8	101
80	Collective variables for the study of long-time kinetics from molecular trajectories: theory and methods. Current Opinion in Structural Biology, 2017, 43, 141-147.	5.7	116
81	Predicting the Kinetics of RNA Oligonucleotides Using Markov State Models. Journal of Chemical Theory and Computation, 2017, 13, 926-934.	5.3	26
82	Mechanistic Models of Chemical Exchange Induced Relaxation in Protein NMR. Journal of the American Chemical Society, 2017, 139, 200-210.	13.7	35
83	Protein-peptide association kinetics beyond the seconds timescale from atomistic simulations. Nature Communications, 2017, 8, 1095.	12.8	137
84	Combining experimental and simulation data of molecular processes via augmented Markov models. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 8265-8270.	7.1	93
85	An efficient multi-scale Greenâ€™s function reaction dynamics scheme. Journal of Chemical Physics, 2017, 147, 184106.	3.0	17
86	Complete proteinâ€“protein association kinetics in atomic detail revealed by molecular dynamics simulations and Markov modelling. Nature Chemistry, 2017, 9, 1005-1011.	13.6	304
87	Variational tensor approach for approximating the rare-event kinetics of macromolecular systems. Journal of Chemical Physics, 2016, 144, 054105.	3.0	53
88	Multiensemble Markov models of molecular thermodynamics and kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E3221-30.	7.1	173
89	Nanoscopic compartmentalization of membrane protein motion at the axon initial segment. Journal of Cell Biology, 2016, 215, 37-46.	5.2	99
90	MHC class II complexes sample intermediate states along the peptide exchange pathway. Nature Communications, 2016, 7, 13224.	12.8	40

#	Article	IF	Citations
91	Commute Maps: Separating Slowly Mixing Molecular Configurations for Kinetic Modeling. Journal of Chemical Theory and Computation, 2016, 12, 5620-5630.	5.3	47
92	Hierarchical Time-Lagged Independent Component Analysis: Computing Slow Modes and Reaction Coordinates for Large Molecular Systems. Journal of Chemical Theory and Computation, 2016, 12, 6118-6129.	5.3	57
93	Molecular dynamics simulations data of the twenty encoded amino acids in different force fields. Data in Brief, 2016, 7, 582-590.	1.0	17
94	HTMD: High-Throughput Molecular Dynamics for Molecular Discovery. Journal of Chemical Theory and Computation, 2016, 12, 1845-1852.	5.3	343
95	Projected metastable Markov processes and their estimation with observable operator models. Journal of Chemical Physics, 2015, 143, 144101.	3.0	15
96	Estimation and uncertainty of reversible Markov models. Journal of Chemical Physics, 2015, 143, 174101.	3.0	102
97	Higher-Order Architecture of Rhodopsin in Intact Photoreceptors and Its Implication for Phototransduction Kinetics. Structure, 2015, 23, 628-638.	3.3	105
98	Response to Comment â€œTransient Complexes between Dark Rhodopsin and Transducin: Circumstantial Evidence or Physiological Necessity?â€•byÂD. Dellâ€™Orco and K.-W. Koch. Biophysical Journal, 2015, 108, 778-779.	0.5	3
99	ReaDDyMM: Fast Interacting Particle Reaction-Diffusion Simulations Using Graphical Processing Units. Biophysical Journal, 2015, 108, 457-461.	0.5	30
100	Beating the Millisecond Barrier in Molecular Dynamics Simulations. Biophysical Journal, 2015, 108, 228-229.	0.5	22
101	Protein conformational plasticity and complex ligand-binding kinetics explored by atomistic simulations and Markov models. Nature Communications, 2015, 6, 7653.	12.8	344
102	Shedding Light on the Dockâ€“Lock Mechanism in Amyloid Fibril Growth Using Markov State Models. Journal of Physical Chemistry Letters, 2015, 6, 1076-1081.	4.6	35
103	Dynamic properties of force fields. Journal of Chemical Physics, 2015, 142, 084101.	3.0	70
104	Gaussian Markov transition models of molecular kinetics. Journal of Chemical Physics, 2015, 142, 084104.	3.0	14
105	A Basis Set for Peptides for the Variational Approach to Conformational Kinetics. Journal of Chemical Theory and Computation, 2015, 11, 3992-4004.	5.3	25
106	PyEMMA 2: A Software Package for Estimation, Validation, and Analysis of Markov Models. Journal of Chemical Theory and Computation, 2015, 11, 5525-5542.	5.3	876
107	Crystal structure of the dynamin tetramer. Nature, 2015, 525, 404-408.	27.8	115
108	Kinetic Distance and Kinetic Maps from Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2015, 11, 5002-5011.	5.3	173

#	Article	IF	Citations
109	Investigating Molecular Kinetics by Variationally Optimized Diffusion Maps. Journal of Chemical Theory and Computation, 2015, 11, 5947-5960.	5.3	54
110	Dynamical Organization of Syntaxin-1A at the Presynaptic Active Zone. PLoS Computational Biology, 2015, 11, e1004407.	3.2	65
111	Statistically optimal analysis of state-discretized trajectory data from multiple thermodynamic states. Journal of Chemical Physics, 2014, 141, 214106.	3.0	73
112	xTRAM: Estimating Equilibrium Expectations from Time-Correlated Simulation Data at Multiple Thermodynamic States. Physical Review X, 2014, 4, .	8.9	25
113	Spectral Rate Theory for Two-State Kinetics. Physical Review X, 2014, 4, .	8.9	16
114	Simulation tools for particle-based reaction-diffusion dynamics in continuous space. BMC Biophysics, 2014, 7, 11.	4.4	74
115	Variational Approach to Molecular Kinetics. Journal of Chemical Theory and Computation, 2014, 10, 1739-1752.	5.3	256
116	Complex RNA Folding Kinetics Revealed by Single-Molecule FRET and Hidden Markov Models. Journal of the American Chemical Society, 2014, 136, 4534-4543.	13.7	84
117	Explicit Spatiotemporal Simulation of Receptor-G Protein Coupling in Rod Cell Disk Membranes. Biophysical Journal, 2014, 107, 1042-1053.	0.5	38
118	Markov state models of biomolecular conformational dynamics. Current Opinion in Structural Biology, 2014, 25, 135-144.	5.7	628
119	Optimal Estimation of Free Energies and Stationary Densities from Multiple Biased Simulations. Multiscale Modeling and Simulation, 2014, 12, 25-54.	1.6	21
120	Spatiotemporal control of endocytosis by phosphatidylinositol-3,4-bisphosphate. Nature, 2013, 499, 233-237.	27.8	362
121	Projected and hidden Markov models for calculating kinetics and metastable states of complex molecules. Journal of Chemical Physics, 2013, 139, 184114.	3.0	144
122	A Variational Approach to Modeling Slow Processes in Stochastic Dynamical Systems. Multiscale Modeling and Simulation, 2013, 11, 635-655.	1.6	249
123	Dynamic neutron scattering from conformational dynamics. I. Theory and Markov models. Journal of Chemical Physics, 2013, 139, 175101.	3.0	22
124	Efficient Bayesian estimation of Markov model transition matrices with given stationary distribution. Journal of Chemical Physics, 2013, 138, 164113.	3.0	32
125	Dynamic neutron scattering from conformational dynamics. II. Application using molecular dynamics simulation and Markov modeling. Journal of Chemical Physics, 2013, 139, 175102.	3.0	12
126	Identification of slow molecular order parameters for Markov model construction. Journal of Chemical Physics, 2013, 139, 015102.	3.0	777

#	Article	IF	Citations
127	ReaDDy - A Software for Particle-Based Reaction-Diffusion Dynamics in Crowded Cellular Environments. PLoS ONE, 2013, 8, e74261.	2.5	117
128	Kinetic characterization of the critical step in HIV-1 protease maturation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 20449-20454.	7.1	92
129	EMMA: A Software Package for Markov Model Building and Analysis. Journal of Chemical Theory and Computation, 2012, 8, 2223-2238.	5.3	136
130	Markov models and dynamical fingerprints: Unraveling the complexity of molecular kinetics. Chemical Physics, 2012, 396, 92-107.	1.9	52
131	Mechanisms of Protein-Ligand Association and Its Modulation by Protein Mutations. Biophysical Journal, 2011, 100, 701-710.	0.5	62
132	Markov state models based on milestoning. Journal of Chemical Physics, 2011, 134, 204105.	3.0	184
133	Crystal structure of nucleotide-free dynamin. Nature, 2011, 477, 556-560.	27.8	277
134	Probing molecular kinetics with Markov models: metastable states, transition pathways and spectroscopic observables. Physical Chemistry Chemical Physics, 2011, 13, 16912.	2.8	106
135	Optimal use of data in parallel tempering simulations for the construction of discrete-state Markov models of biomolecular dynamics. Journal of Chemical Physics, 2011, 134, 244108.	3.0	46
136	Dynamical fingerprints for probing individual relaxation processes in biomolecular dynamics with simulations and kinetic experiments. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 4822-4827.	7.1	105
137	Dynamical reweighting: Improved estimates of dynamical properties from simulations at multiple temperatures. Journal of Chemical Physics, 2011, 134, 244107.	3.0	55
138	Markov models of molecular kinetics: Generation and validation. Journal of Chemical Physics, 2011, 134, 174105.	3.0	968
139	Optimal Identification of Semi-Rigid Domains in Macromolecules from Molecular Dynamics Simulation. PLoS ONE, 2010, 5, e10491.	2.5	21
140	Probability distributions of molecular observables computed from Markov models. II. Uncertainties in observables and their time-evolution. Journal of Chemical Physics, 2010, 133, 105102.	3.0	38
141	On the Approximation Quality of Markov State Models. Multiscale Modeling and Simulation, 2010, 8, 1154-1177.	1.6	160
142	Estimating the sampling error: Distribution of transition matrices and functions of transition matrices for given trajectory data. Physical Review E, 2009, 80, 021106.	2.1	40
143	Constructing the equilibrium ensemble of folding pathways from short off-equilibrium simulations. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 19011-19016.	7.1	730
144	Probability distributions of molecular observables computed from Markov models. Journal of Chemical Physics, 2008, 128, 244103.	3.0	123

#	Article	IF	Citations
145	Data-based parameter estimation of generalized multidimensional Langevin processes. Physical Review E, 2007, 76, 016706.	2.1	43
146	Hierarchical analysis of conformational dynamics in biomolecules: Transition networks of metastable states. Journal of Chemical Physics, 2007, 126, 155102.	3.0	363
147	Transition Networks for the Comprehensive Characterization of Complex Conformational Change in Proteins. Journal of Chemical Theory and Computation, 2006, 2, 840-857.	5.3	88
148	Automated computation of low-energy pathways for complex rearrangements in proteins: Application to the conformational switch of Ras p21. Proteins: Structure, Function and Bioinformatics, 2005, 59, 534-544.	2.6	34
149	Computational tools for analysing structural changes in proteins in solution. Applied Bioinformatics, 2003, 2, S11-7.	1.6	0